



Incorporating Reality Into Process Simulation

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Levels of Reality in Process Simulation

- 1. Data Accuracy and Comprehensiveness**
 - Physical Properties
 - Phase Properties (BIP's)
 - Chemical Properties
- 2. Equilibrium Models**
 - Phase (VLE, LLE, SLE)
 - Chemical Reaction (Gibbs or Emperical)
- 3. Rate Models**
 - Reaction
 - Mass Transfer
 - Heat Transfer
 - Momentum Transfer (pressure drops)



Levels of Reality in Process Simulation

4. Mechanical Considerations

- **Pump and Compressor performance curves**
- **Valve Geometry**
- **Solids UnitOps**

5. Time Dependence

- **Holdups**
- **Transients inputs and fluctuations**
- **Signal delays**
- **Control response**



Historically,

**Steady State
Process
Simulation**

**Equipment
Sizing
& Rating**

**Reactor
Design**

**Training
Simulators**

**Dynamic
Process
Simulation**

**Plant
Optimization**



Historically,

Over time these gaps began to close:

- i. Faster computers**
- ii. Better software technology**
- iii. Improved numerical techniques**
- iv. Better engineering models**
- v. Cumulative effort**

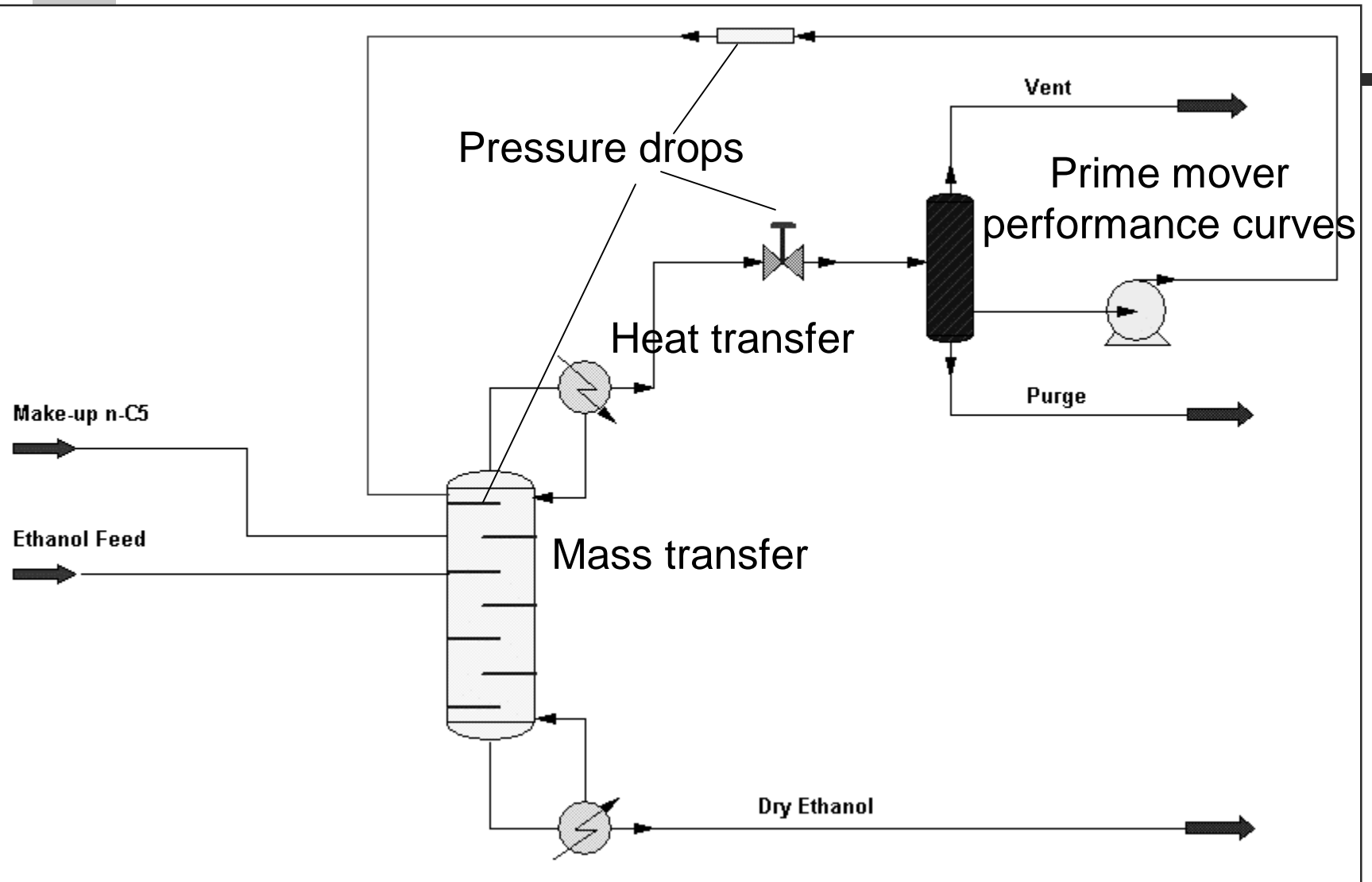


Historically,

These things resulted in the following developments:

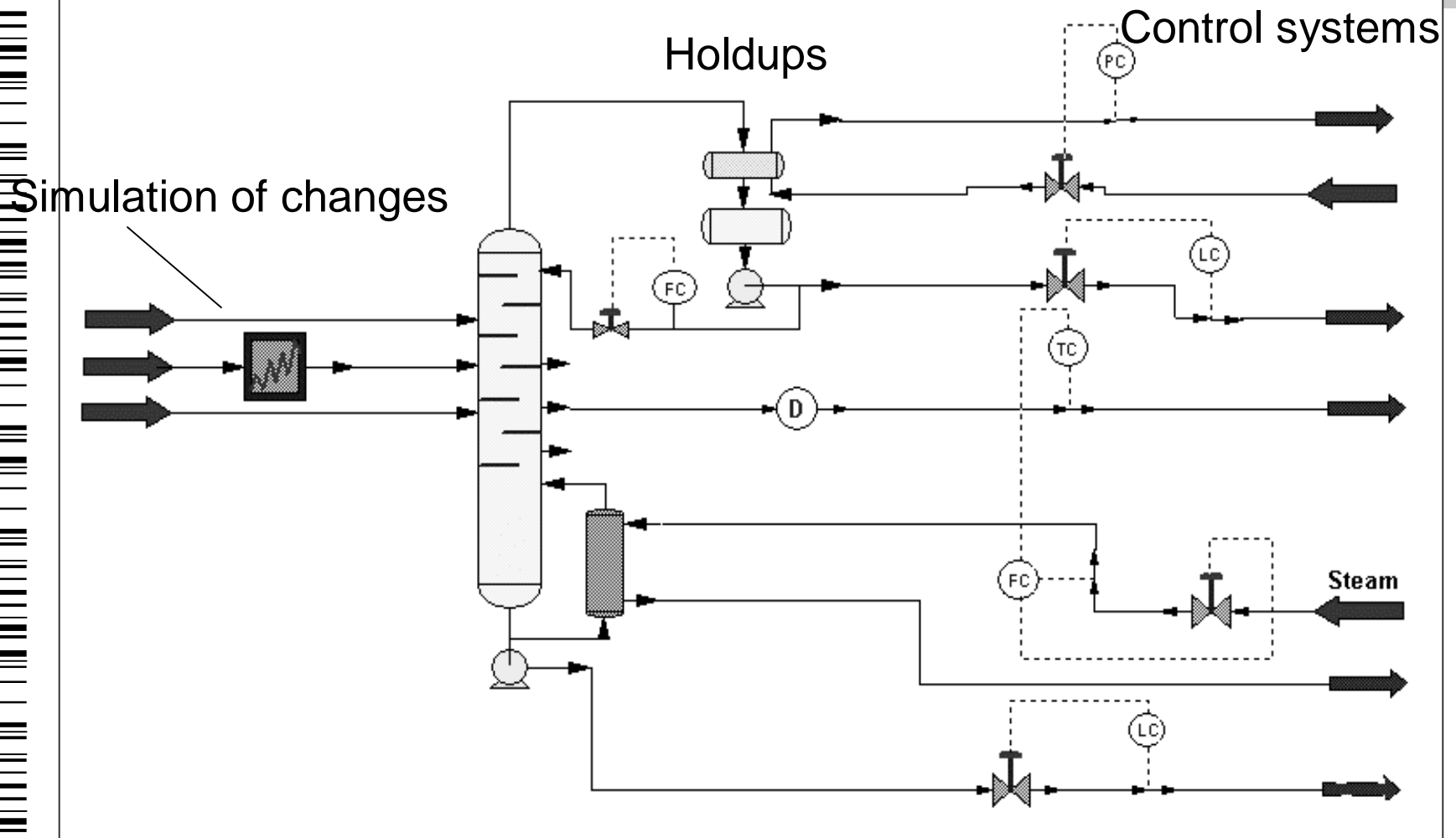
- **Dynamic Simulation**
 - required equipment parameters such as geometry, Cv, PIDC, etc
- **Mass transfer**
 - required column geometries
- **Numerical techniques**
 - full or quasi equation solving permitted integration of piping, valves, etc.
- **Better software and faster computers**
 - integration of many components or models
 - customization
 - communications

Now simulations can be more realistic:

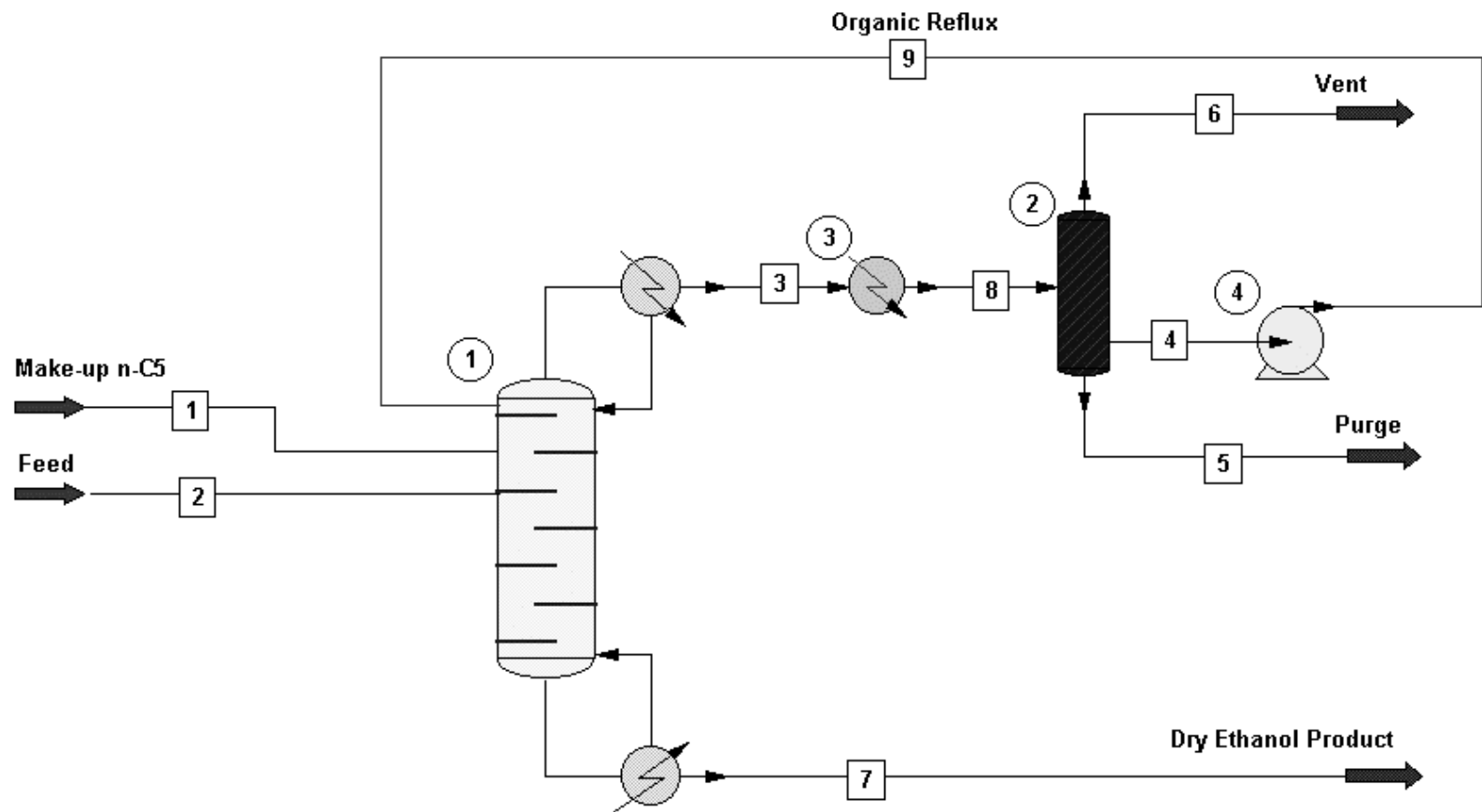


Now simulations can be more realistic:

Dynamic considerations

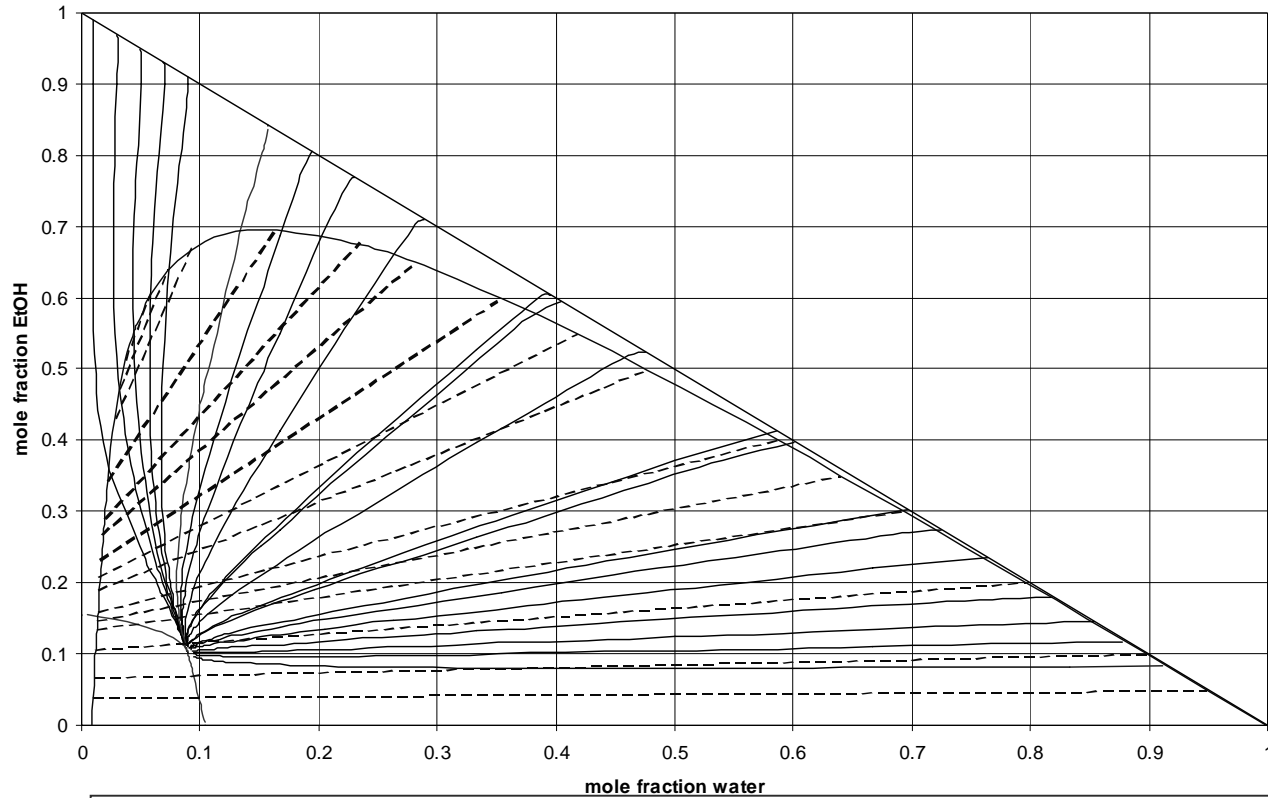


Azeotropic Distillation Example:



Residue Curve Map for Azeotropic System

Residue Map for EtOH-H₂O-nC₅ System



From this map we can verify our thermodynamic model.

	Miscible/immiscible	Azeotrope composition, mole%	Azeotrope temperature, F
Ethanol-water	Miscible	90.4 .v. 90.8 EtOH	172.8 .v. 173.1
Ethanol-npentane	Miscible	92.4 .v. 92.2 nC ₅	93.7 .v. 95.5
npentane-water	Immiscible	94.6 .v. 94.6 nC ₅	94.3 .v. 93.8
Ethanol-water-npentane	immiscible	4.4,6.1,89.5 .v. 4.9,5.4,89.7	92.1 .v. 93.2

Preliminary Material Balance prepared from Residue Map

Organic reflux
796.3 lbmoles/hr nC5
114.0 lbmoles/hr EtOH
11.9 lbmoles/hr H2O

Make-up n-C5

Feed

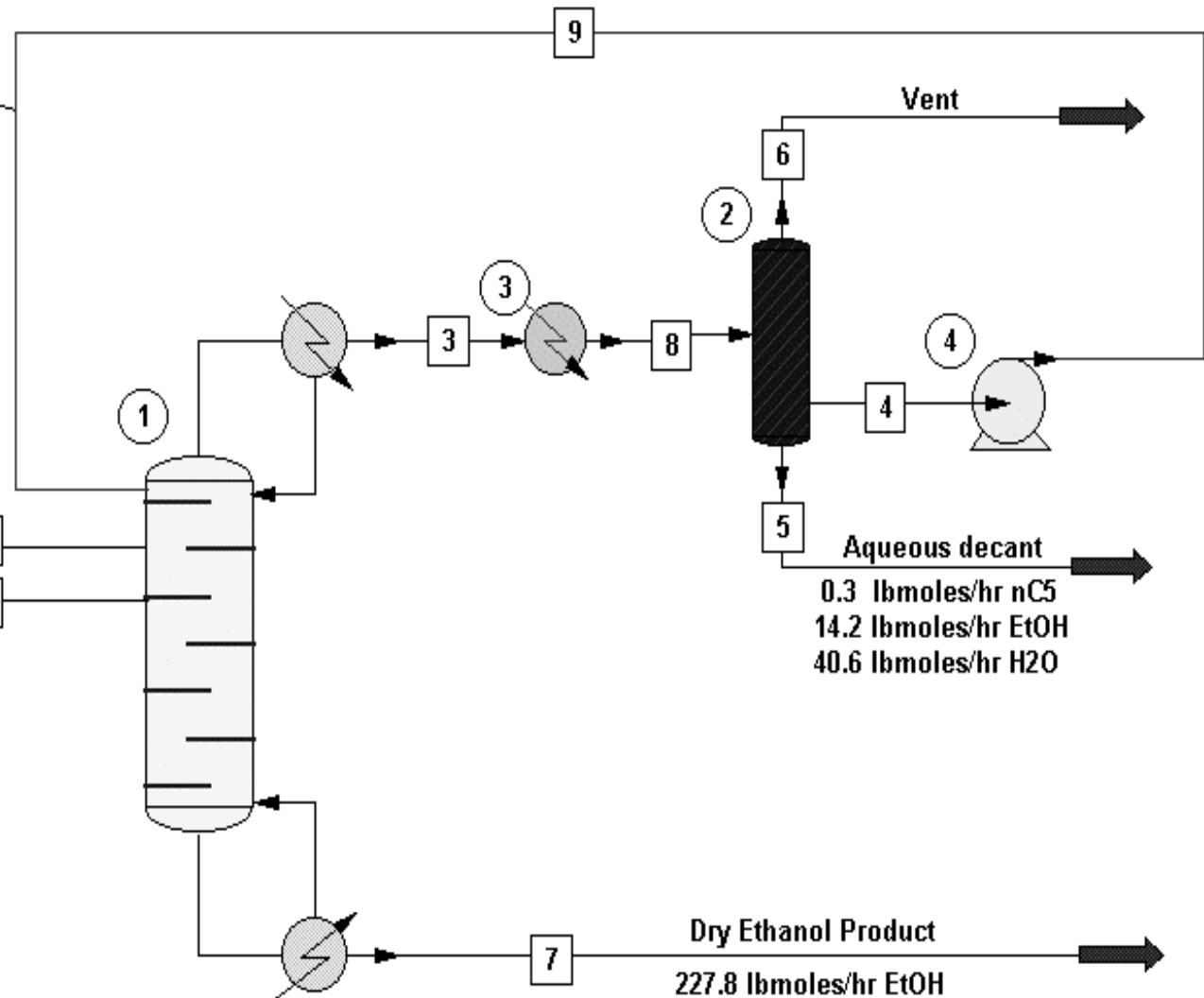
242.0 lbmoles/hr EtOH
40.6 lbmoles/hr H2O

Vent

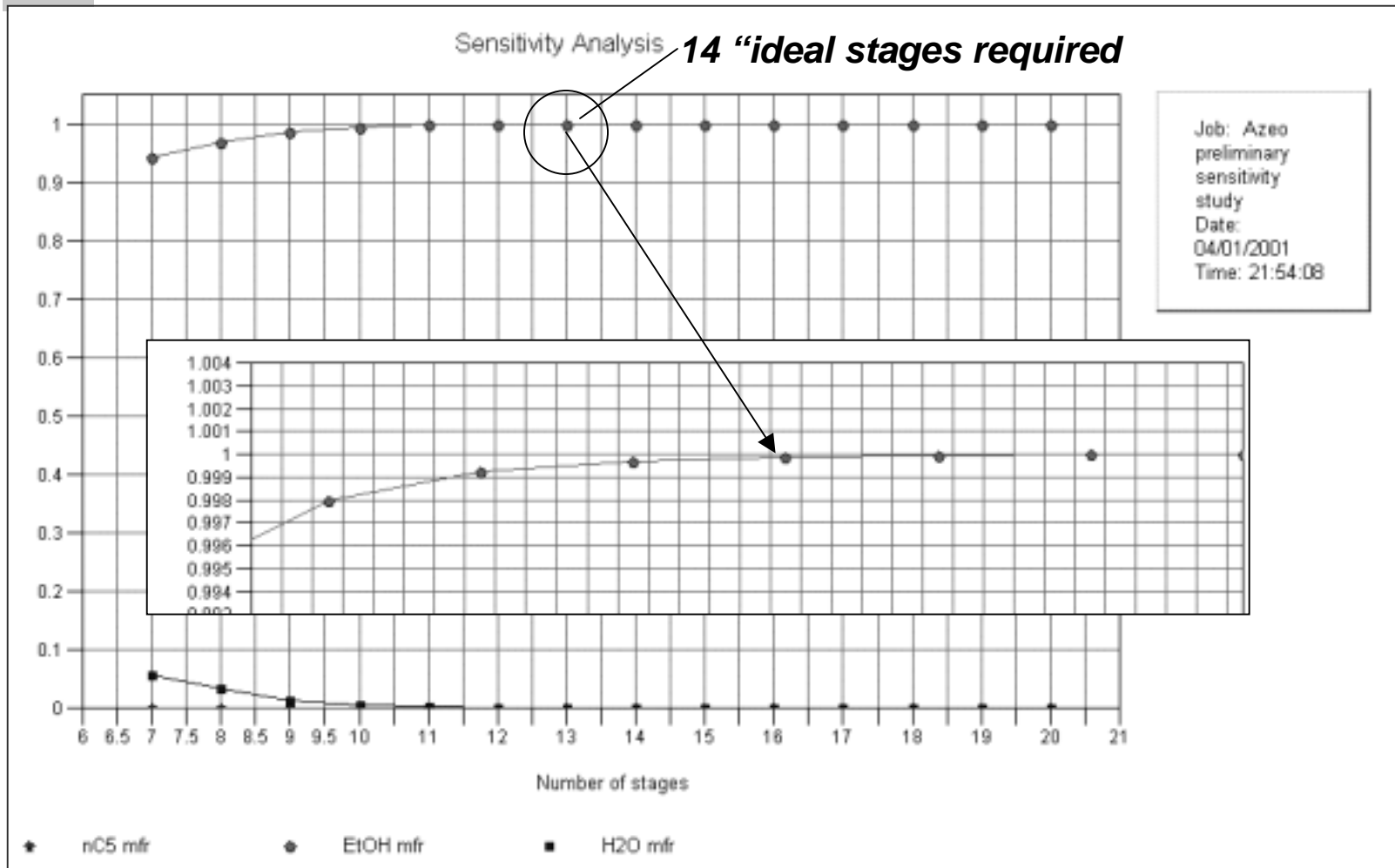
Aqueous decant

0.3 lbmoles/hr nC5
14.2 lbmoles/hr EtOH
40.6 lbmoles/hr H2O

Dry Ethanol Product
227.8 lbmoles/hr EtOH



Sensitivity analysis using equilibrium stages:





Mass Transfer in Distillation Calculations

The Early History of Distillation Calculations

- 1. Concept of equilibrium stage introduced by Sorel in 1893.**
- 2. McCabe-Thiele diagrams for number of theoretical stages in 1925**
- 3. Lewis-Matheson and Thiele-Geddes methods for rigorous (tray-by-tray) multicomponent distillation in 1930's. Not generally used until the appearance of computers in the 1950's.**



Mass Transfer in Distillation Calculations (cont.)

In all of these methods the departure from thermodynamic equilibrium is accounted for by using empirical factors:

- (i) stages efficiencies for trays**
- (ii) HETP for packing**

Trays: Stage efficiencies can vary $-\infty$ to $+\infty$. Vary with component, stage, conditions, etc.

Packing: HETP varies not only with size and type of packing, but also from one component to another and strongly from point to point in a column to another.

These phenomena are especially true for non-ideal mixtures, operating at extreme conditions.



Mass Transfer in Distillation Calculations (cont.)



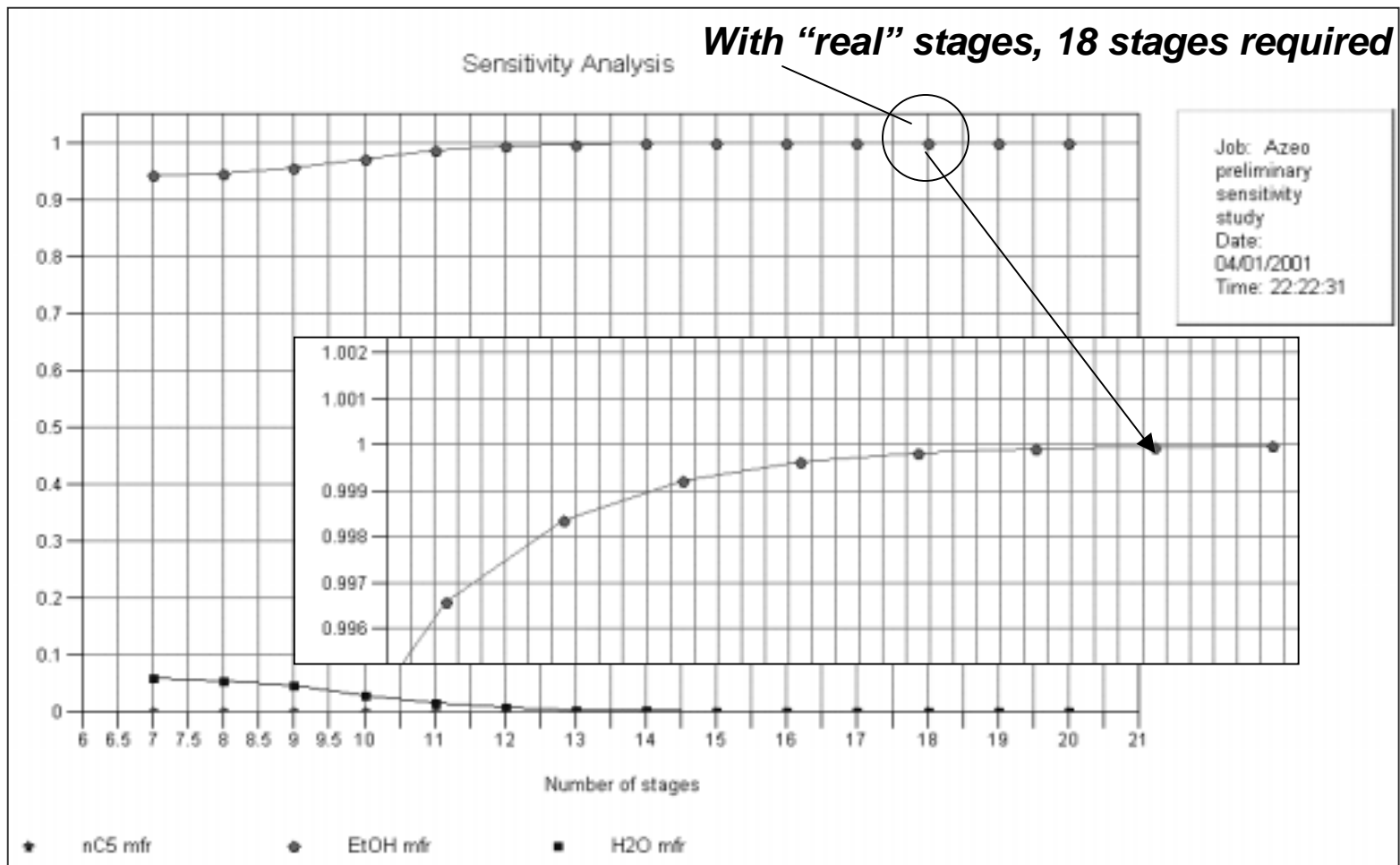
The rate based approach:

- 1. Is more complex.**
- 2. Has shorter application history.**
- 3. Is completely predictive (based on component physical properties and BIPs), so avoids stage efficiencies and HETP.**
- 4. Is at least as accurate as the equilibrium method.**
- 5. Is the only method which can guarantee the accuracy of simulations involving simultaneous mass transfer and chemical reactions.**

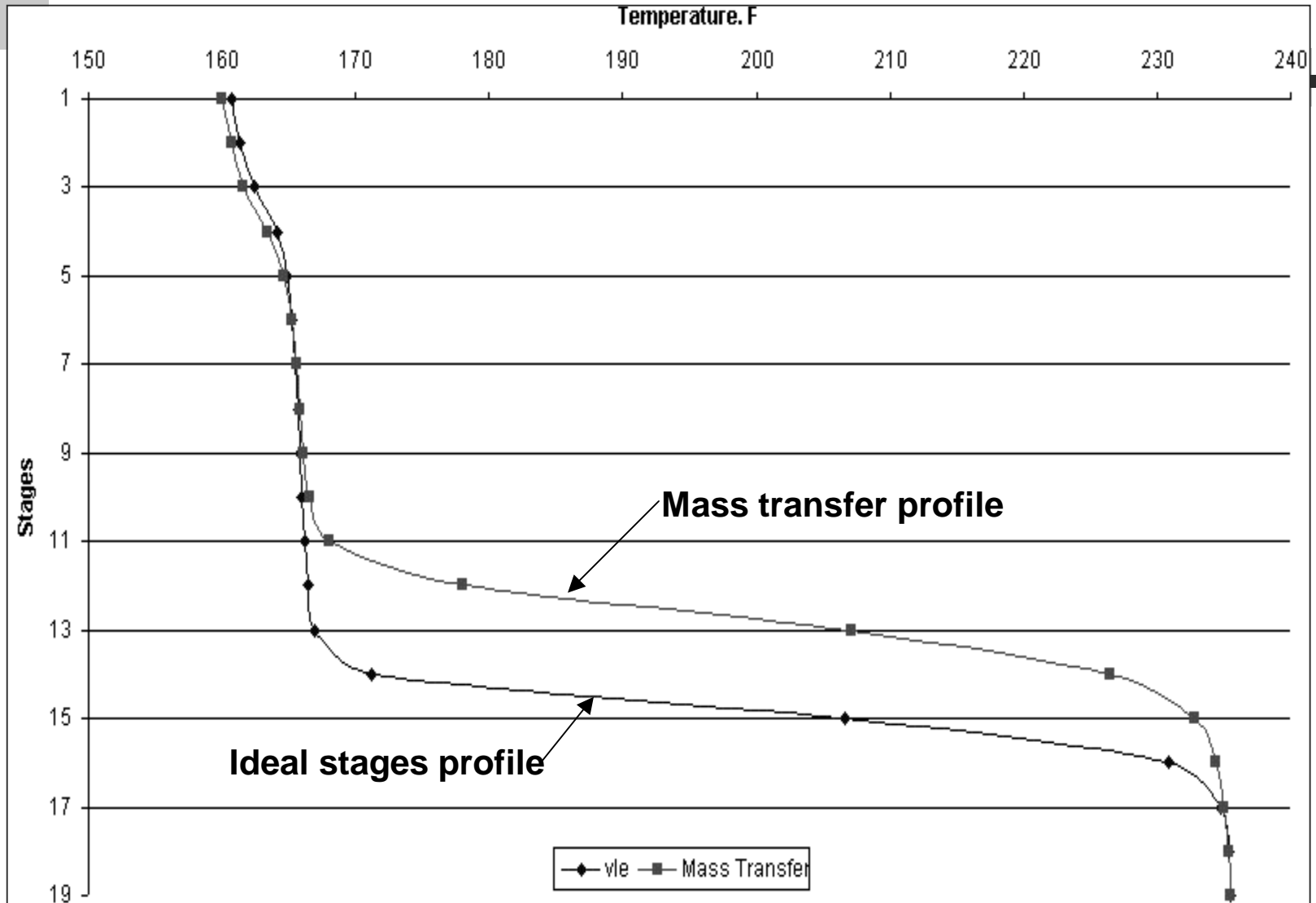
With tray layout and mass transfer calculations included:

Equip.	1	Tray No.	1
Tray Loadings		Vapor	Liquid
		64176.582 lb/h	62944.359 lb/h
		124535.495 ft ³ /hr	1723.614 ft ³ /hr
Density		0.515 lb/ft ³	36.519 lb/ft ³
System factor		1.000
Valve type	:	V-1	
Valve material	:	S.S.	
Valve thickness, gage		12.000
Deck thickness, gage		14.000
Tower internal diameter, ft		6.000
Tray spacing, in		24.000
No. of tray liquid passes		1
Downcomer dimension,		Width in	Length in
Side		10.750	51.320
Avg. weir length in		51.320
Weir height, in		2.000
Flow path length in		50.500
Flow path width in		65.559
Tray area, ft ²		28.274
Tray active area ft ²		22.991
% flood		47.900
Hole area ft ²		4.360
Approx # of valves		342
Tray press loss, in		3.977
Tray press loss, psi		0.084
Dry press drop, in		2.138
Downcomer clearance in		3.000
Downcomer head loss in		0.130
Downcomer backup in		7.205
Downcomer residence time, sec		3.313
Liquid holdup ft ³		5.110
Liquid holdup lb		186.605
Design pressure, psia		47.558
Joint efficiency		0.850
Allowable stress psia		13700.000

Sensitivity analysis using mass transfer (rate based) method:



Temperature profiles under “ideal” and “real” conditions:





Heat transfer:

In conventional simulations, heat exchangers are simulated by making two types of specifications:

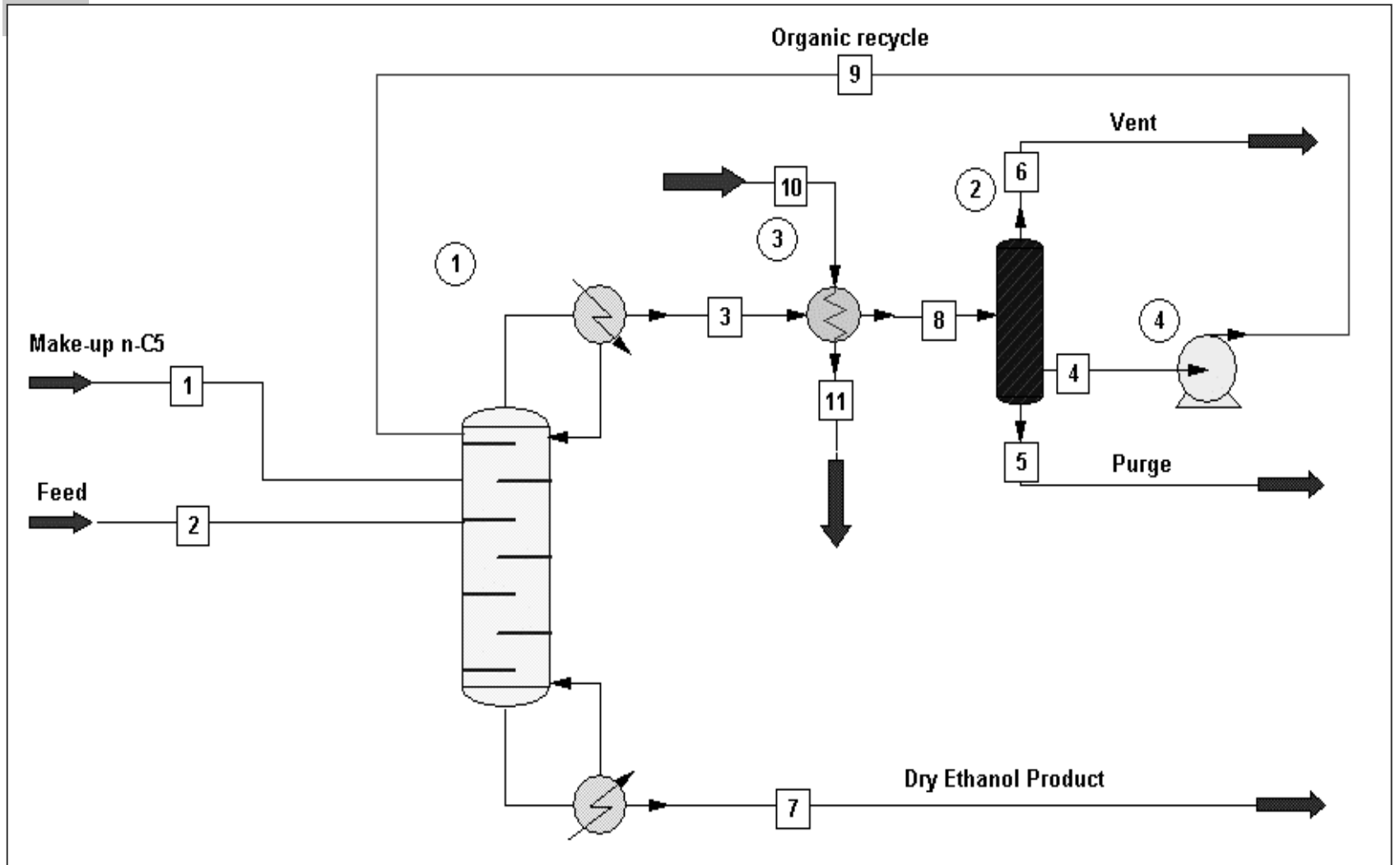
- Thermodynamic specs – T,Q,VF,...
- “Rating” specs – $U \cdot A$ (used frequently in dynamics)

This approach will not account for changing conditions which affect:

- film coefficients
- pressure drops
- varying outlet temperatures
- possible unexpected phase changes

Rigorous rating is done after the simulation.

Heat transfer:

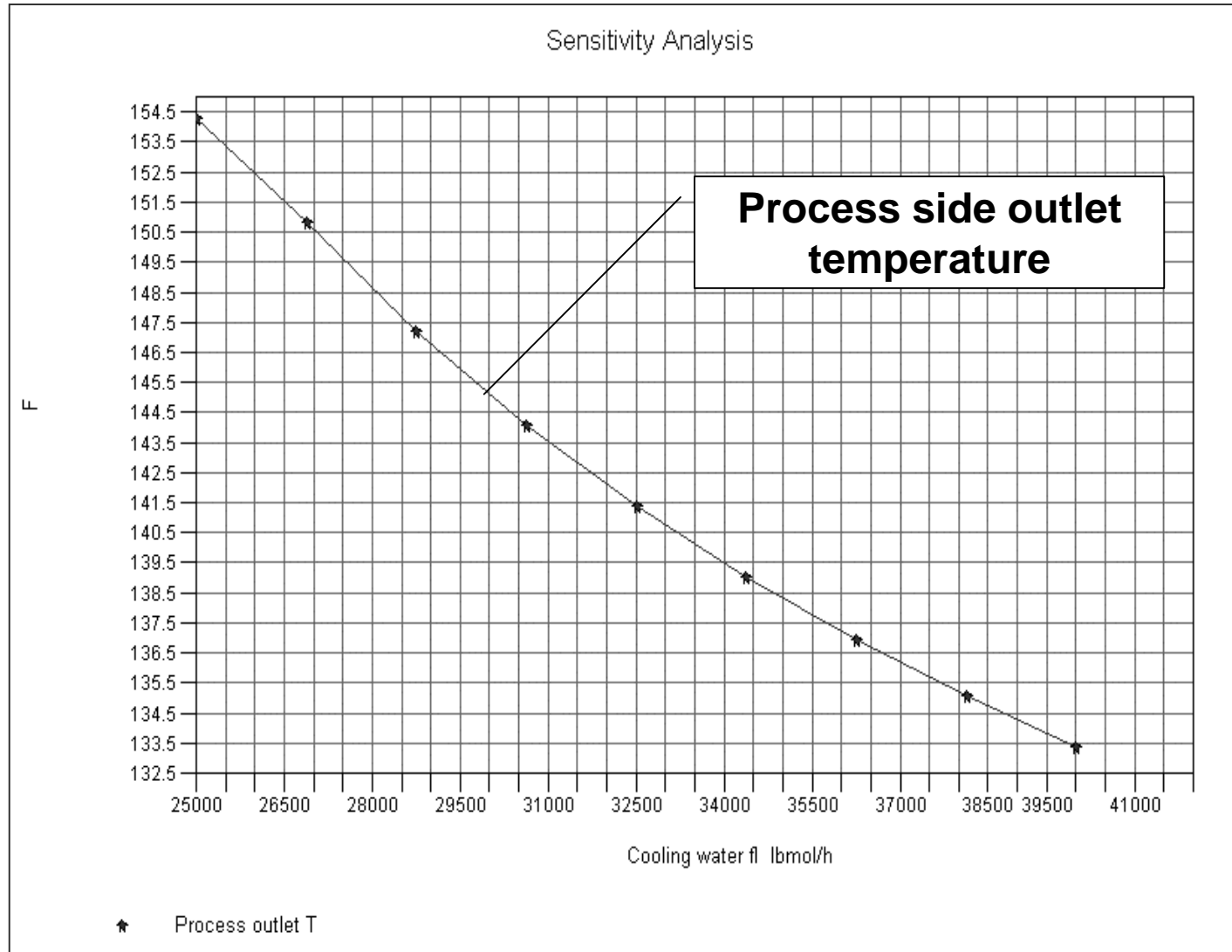


Heat transfer:

TEMA SHEET			

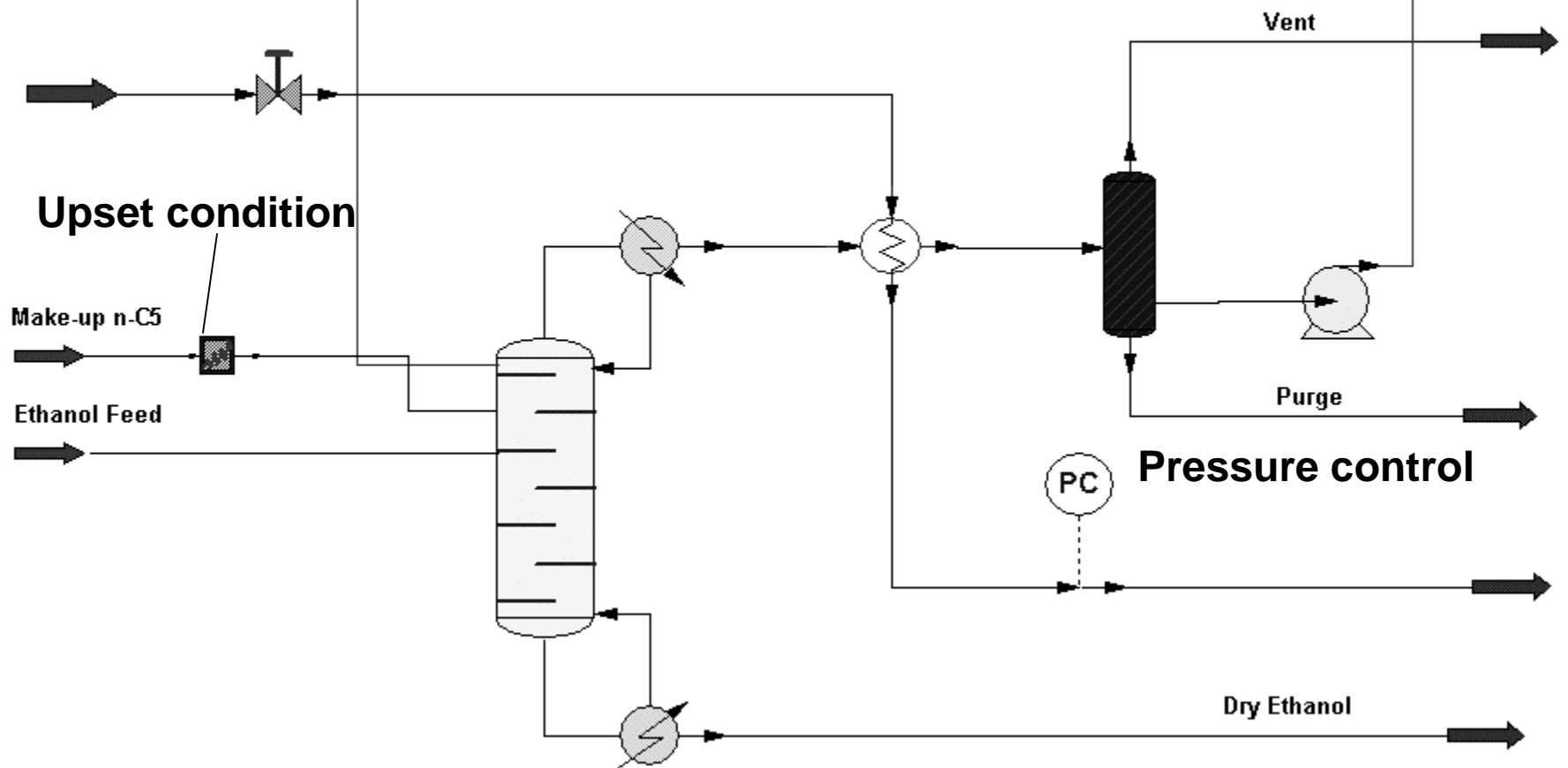
1			
2 Customer		Ref No.	
3 Address		Prop No.	
4 Plant Loc.		Date	Rev
5 Service of Unit		Item	
6 Size 27.0in x 20.0ft Type AEL (Hor/Vert) H Connected in 1 Para 1 Seri			
7 Surf/Unit 2572.2/2536.0 ft2; Shell/Unit 1.000000 Surf/Shell 2572.2/2536.0 ft2			
8	PERFORMANCE OF ONE UNIT		
9 Type of Process	Horiz Cond	Sensible	
10 Fluid Allocation	Shell Side	Tube Side	
11 Fluid Name			
12 Flow	64329.0	229691.2	lb/h
13 Liquid	0.0	229691.2	lb/h
14 Vapor	64329.0	0.0	lb/h
15 NonCondensable	0.00000	0.00000	lb/h
16 Steam	0.0	0.0	lb/h
17 Evap/Cond	64329.0	0.0	lb/h
18 Density	0.507/36.923	0.000/60.874	lb/ft3
19 Conductivity	0.011/0.059	0.000/0.361	Btu/hr-ft-F
20 Specific Heat	0.443/0.625	0.000/0.999	Btu/lb-F
21 Viscosity at Avg.	0.009/0.207	0.000/0.705	cP
22 Latent Heat	169.45	0.00	Btu/lb
23 Temperature(In/Out)	160.217/146.432	80.000/130.883	F
24 Operating Pressure	47.56	50.00	psia
25 Fouling Factor	0.001000	0.001000	hr-ft2-F/Btu
26 Velocity	6.18	0.76	ft/sec
27 Press Drop Allow/Calc	3.500/1.046	5.000/0.066	psi
28 Heat Exchanged 1.166e+001 MMBtu; MYD(Corrected): 48.91 F			
29 Transfer Rate, Service: 94.0 Clean: 115.8 Btu/hr-ft2-F			
30	CONSTRUCTION DATA/SHELL		Sketch
31	Shell Side	Tube Side	
32 Design/Test Press psia	0.000000/Code	0.000000/Code	
33 Design Temperature F	0.000	0.000	
34 No. Passes per Shell	1	1	
35 Corrosion Allowance in	0.000	0.000	
36 Connections TH TH in	1.000	1.000	

Heat transfer:

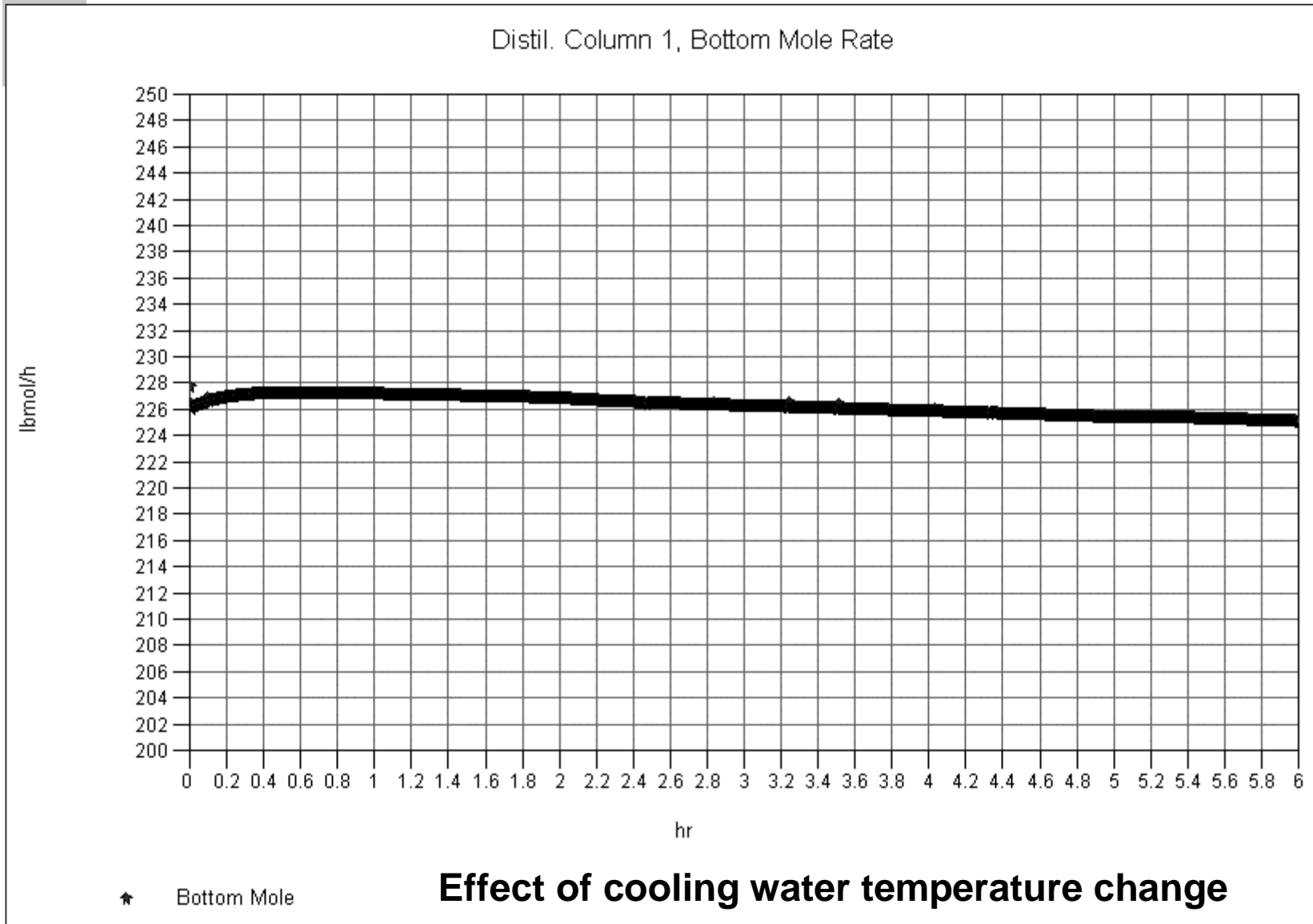


Dynamic Simulation

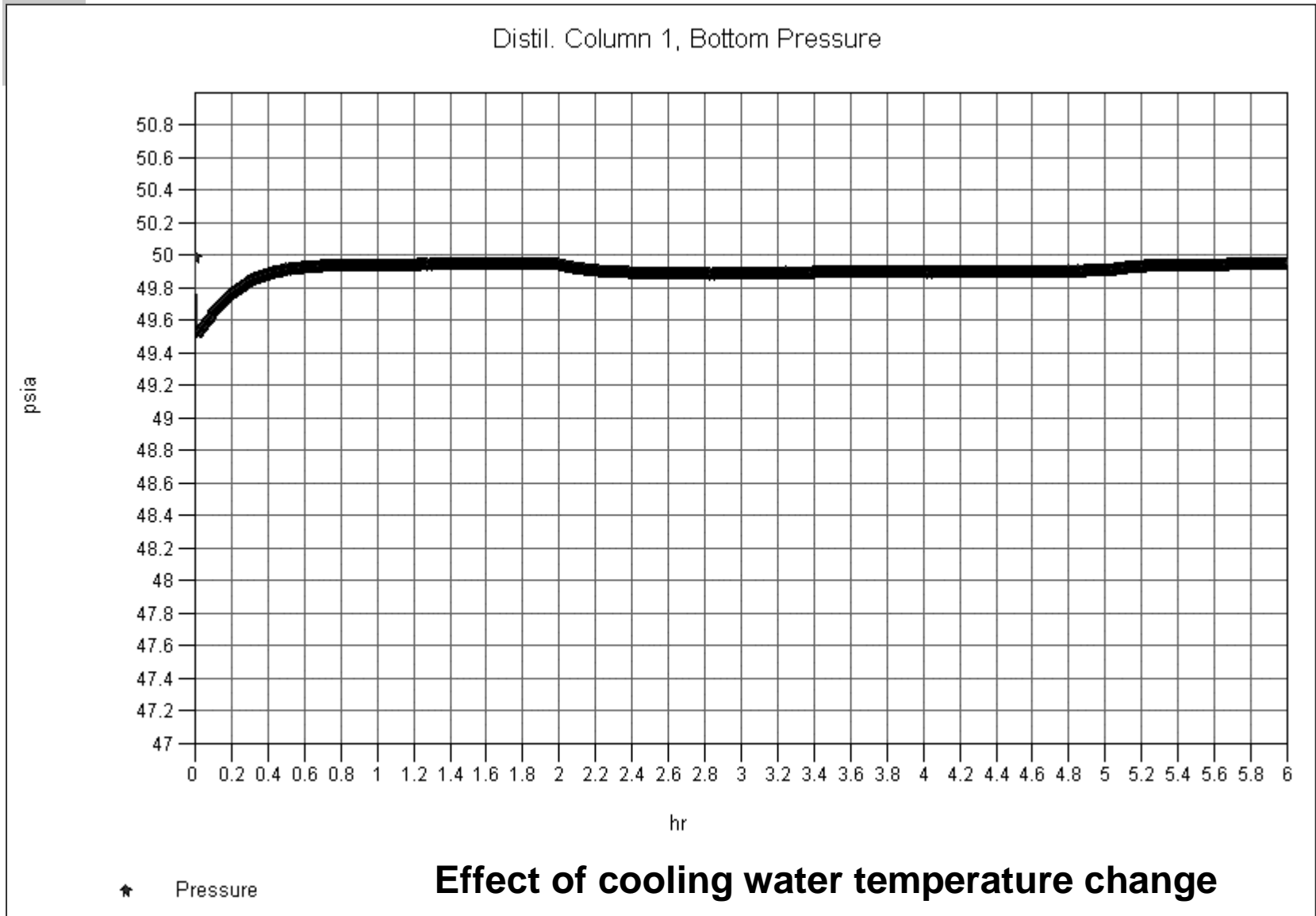
Effect of cooling water temperature change



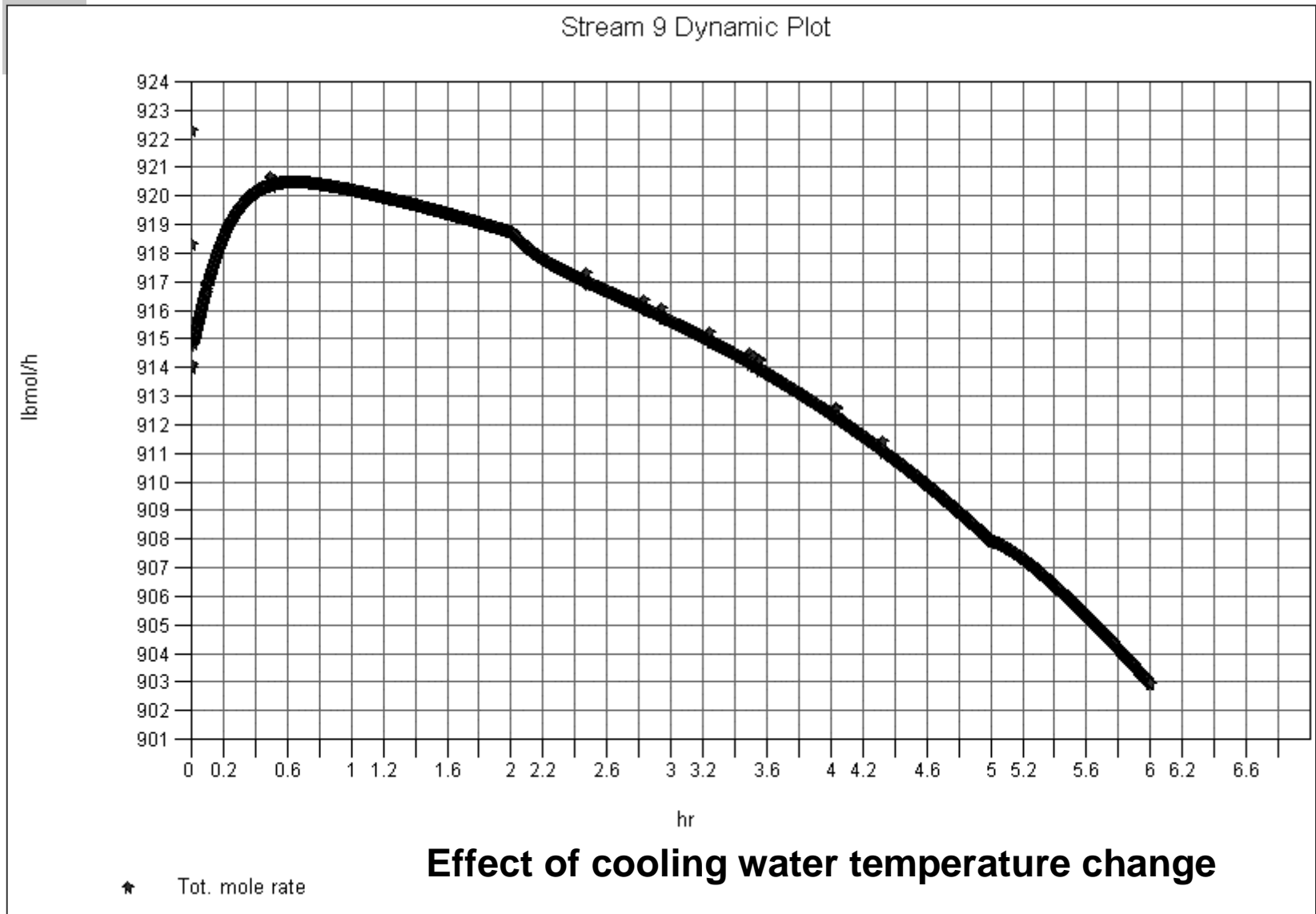
Dynamic Simulation



Dynamic Simulation

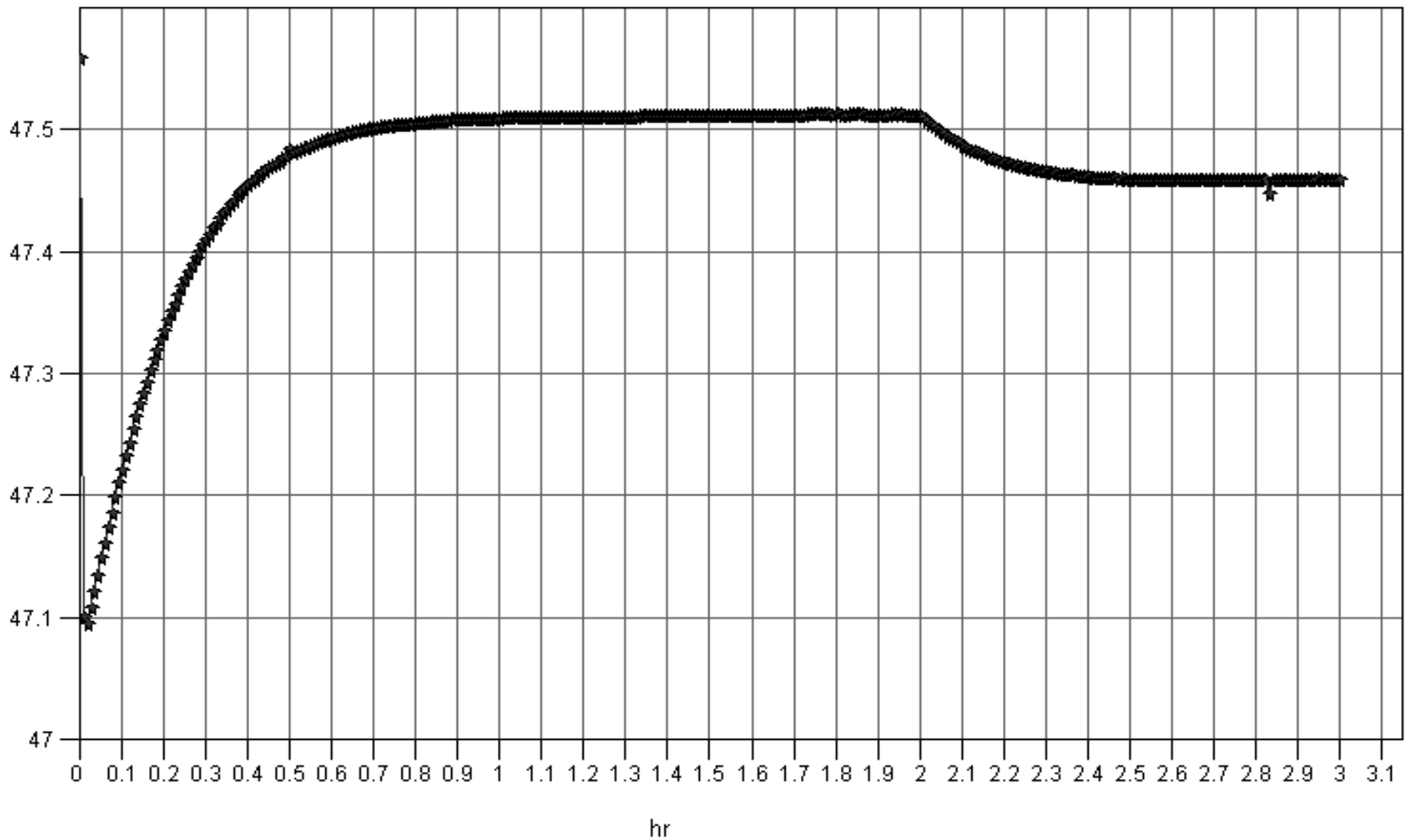


Dynamic Simulation

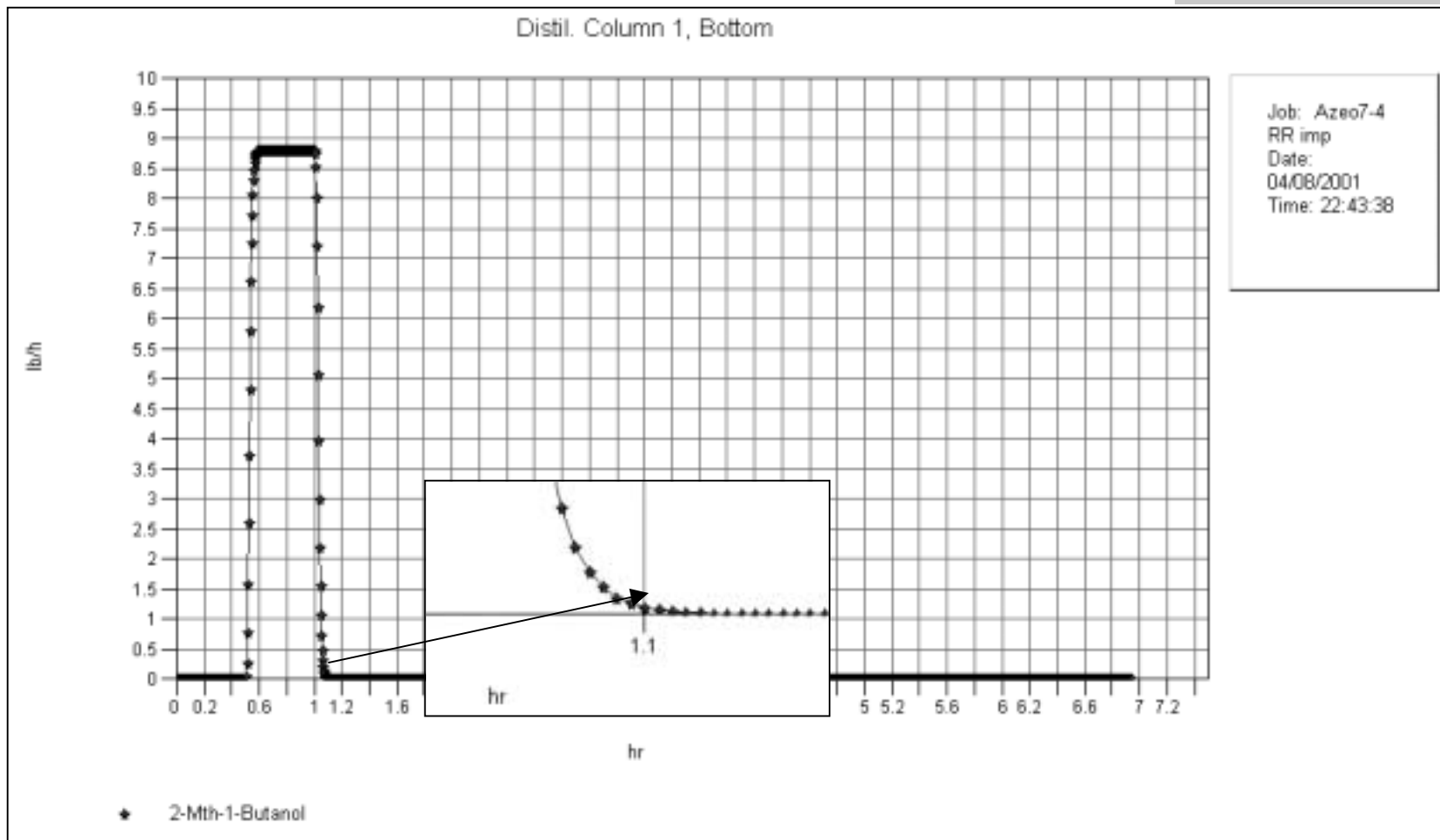


Effect of feed change on column pressure control:

Distil. Column 1, Condenser Pressure



Response to feed impurities:





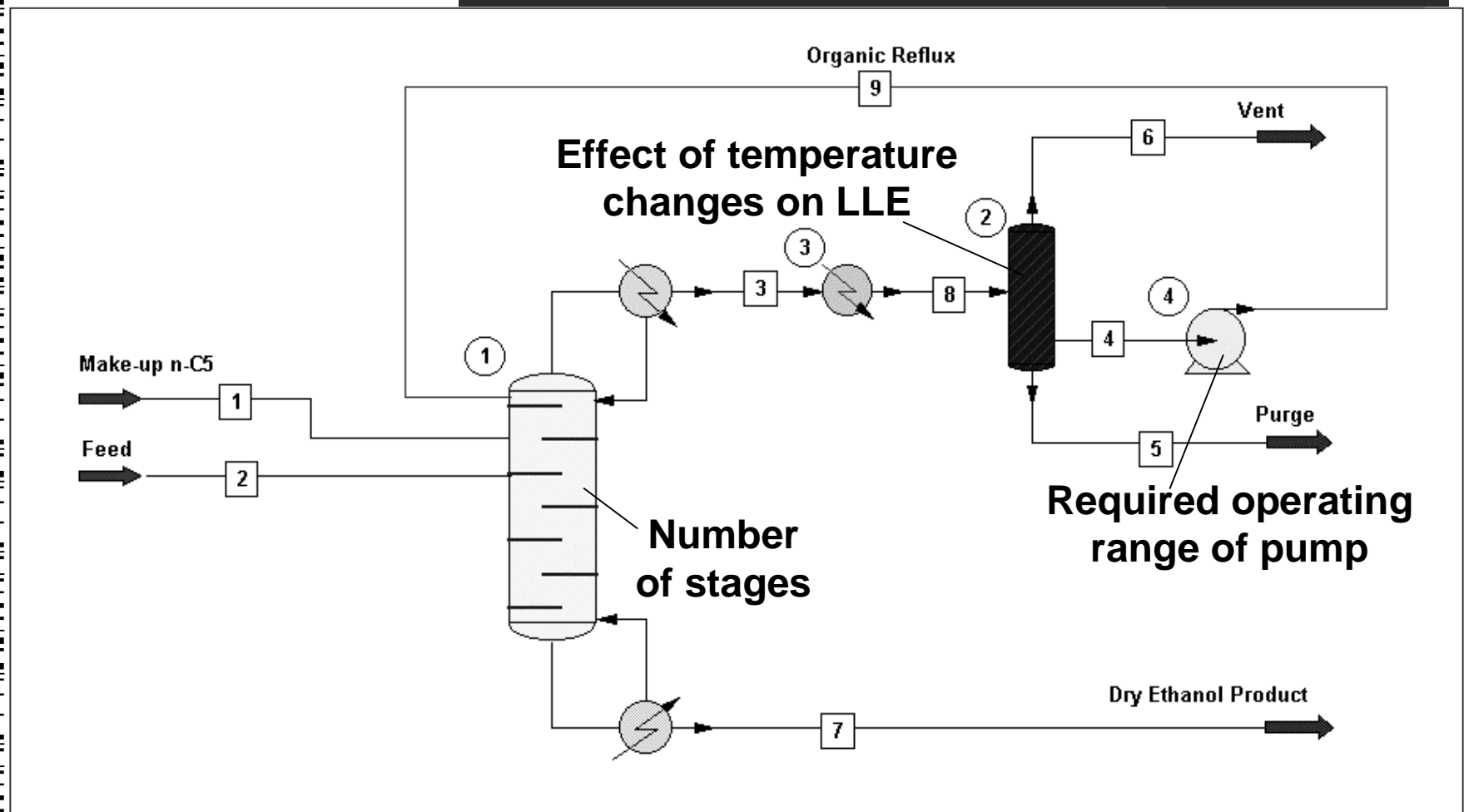
Equipment Which Can Be Included:

- **Distillation**
- **Reactors (CSTR's, PFR's special models)**
- **Heat Exchangers**
- **Prime movers = pumps, compressors, etc.**
- **Pipes**
- **Valves**
- **Vessels and Tanks**
- **PID Controllers**

So

What?

Benefits of “reality” simulations:





Some final notes





Mass Transfer in Distillation Calculations (cont.)

TWO TYPES OF METHODS:

- 1) Methods of the first type begin with the mass and heat balances of an differential element of the packing or of the two-phase layer on the plate.**
- 2) The other group of methods of simulation for multicomponent separation is the non-equilibrium stage model pioneered by Krishnamurty and Taylor.**

Both types of methods give basically the same results. At present, the latter model is the more accepted approach.

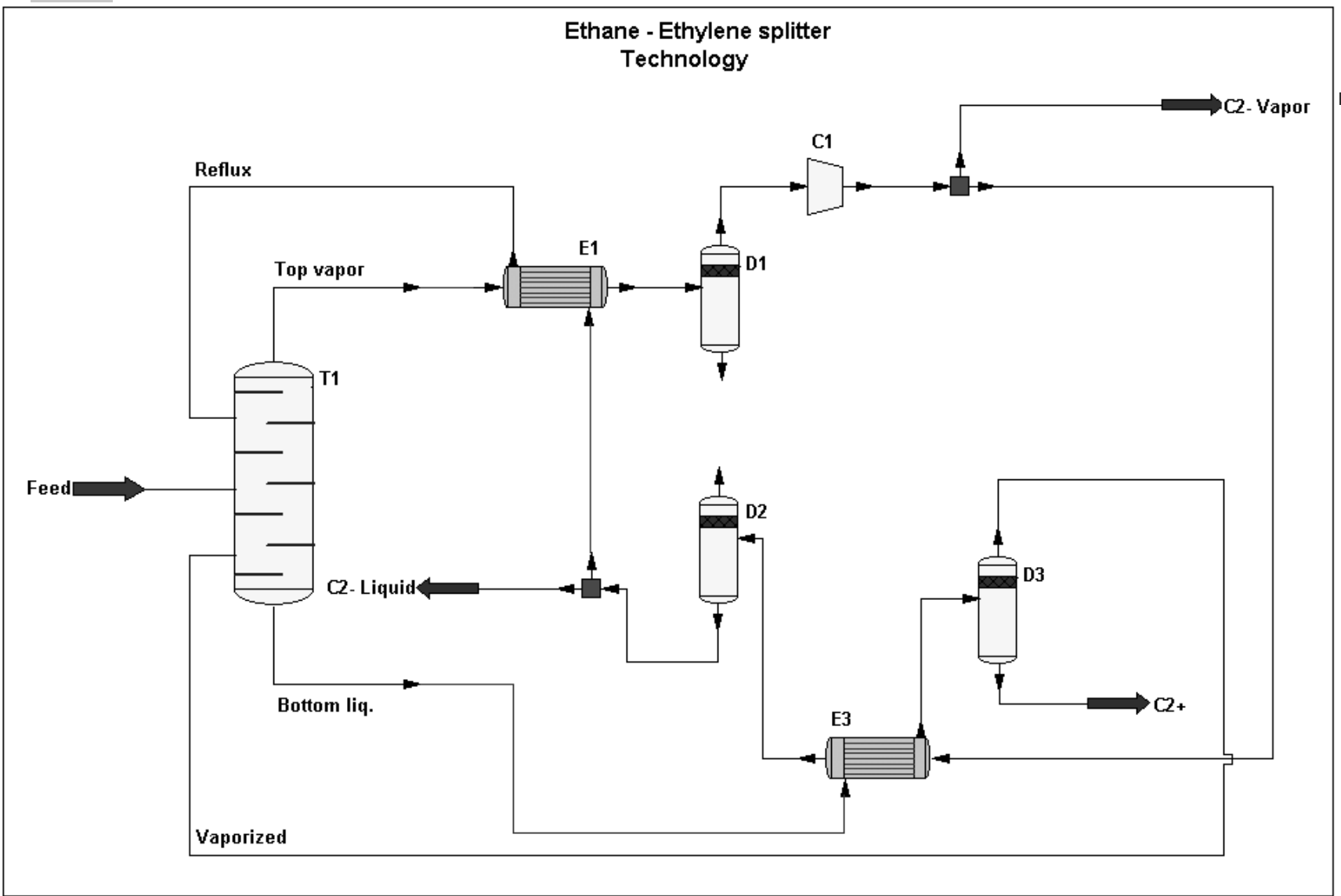


Mass Transfer in Distillation Calculations (cont.)

In this presentation some examples of experimentally verified rated based distillations are presented. The chosen test systems cover a range of components which exhibiting various degrees of differences in chemical structure and in the binary diffusivities and/or enthalpies of vaporization.

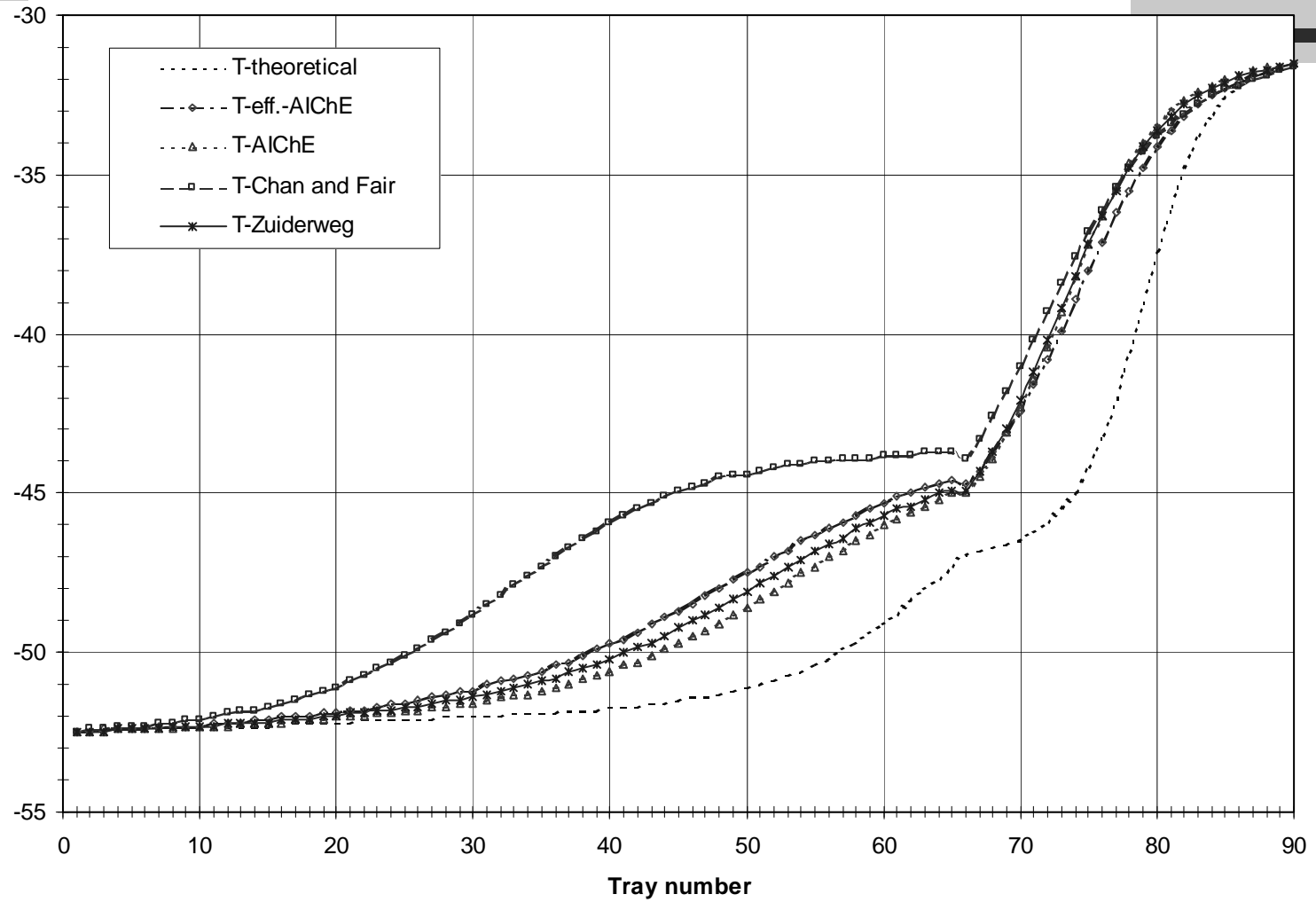
- Ethanol/water/n-pentane**
- Ethane/Ethylene**
- Formaldehyde/water/methanol**
- HCl/water/air**

Ethane - Ethylene splitter Technology

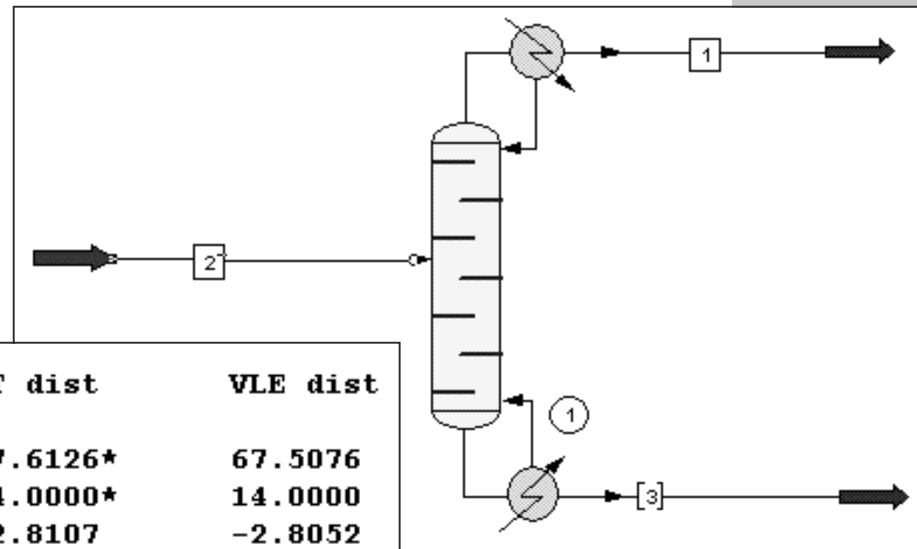


Temperature profiles

Temperature

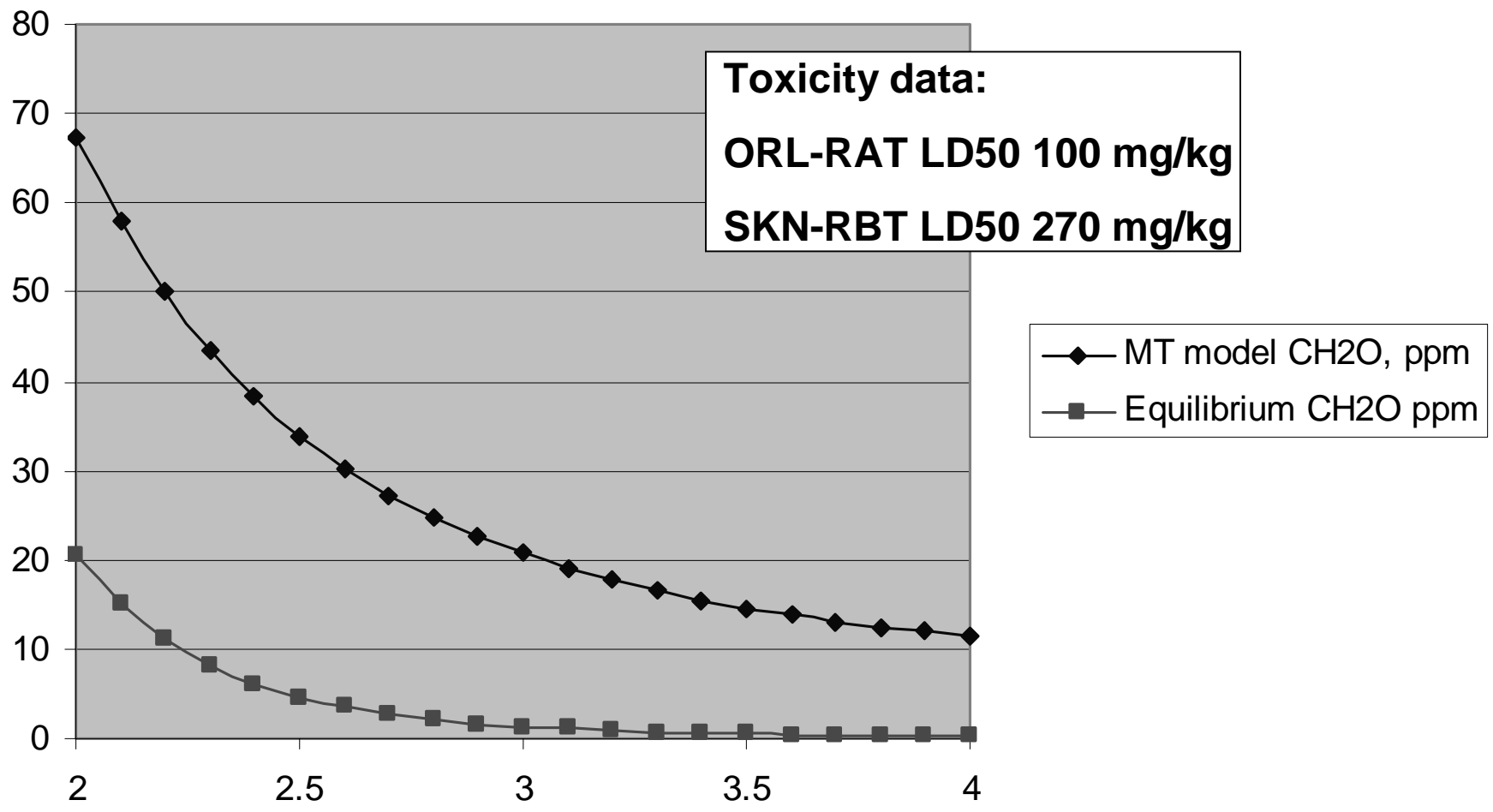


Formaldehyde/Water/Methanol:



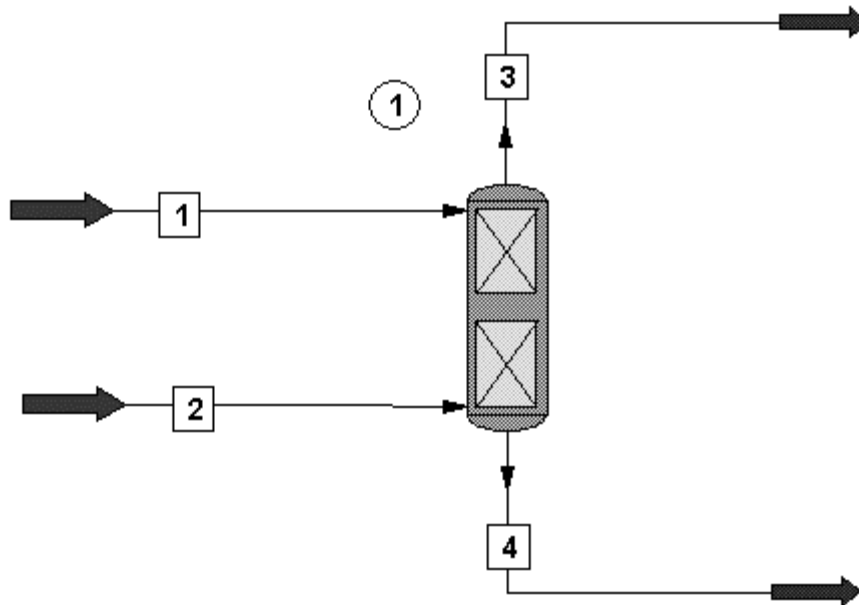
Stream No.	MT dist	VLE dist
Stream Name		
Temp C	67.6126*	67.5076
Pres psia	14.0000*	14.0000
Enth MMBtu/h	-2.8107	-2.8052
Vapor mole fraction	0.00000	0.00000
Total lbmol/h	24.7424	24.7161
Total lb/h	874.3914	875.7383
Total std L gpm	2.0923	2.0970
Total std V scfh	8883.31	8873.87
Component mass fractions		
Water	0.092872	0.089523
Methanol	0.678298	0.682064
Formaldehyde	0.000100	0.000034
N-Butyl Acetate	0.228730	0.228379
Phenol	0.000000	0.000000

Formaldehyde/Water/Methanol:



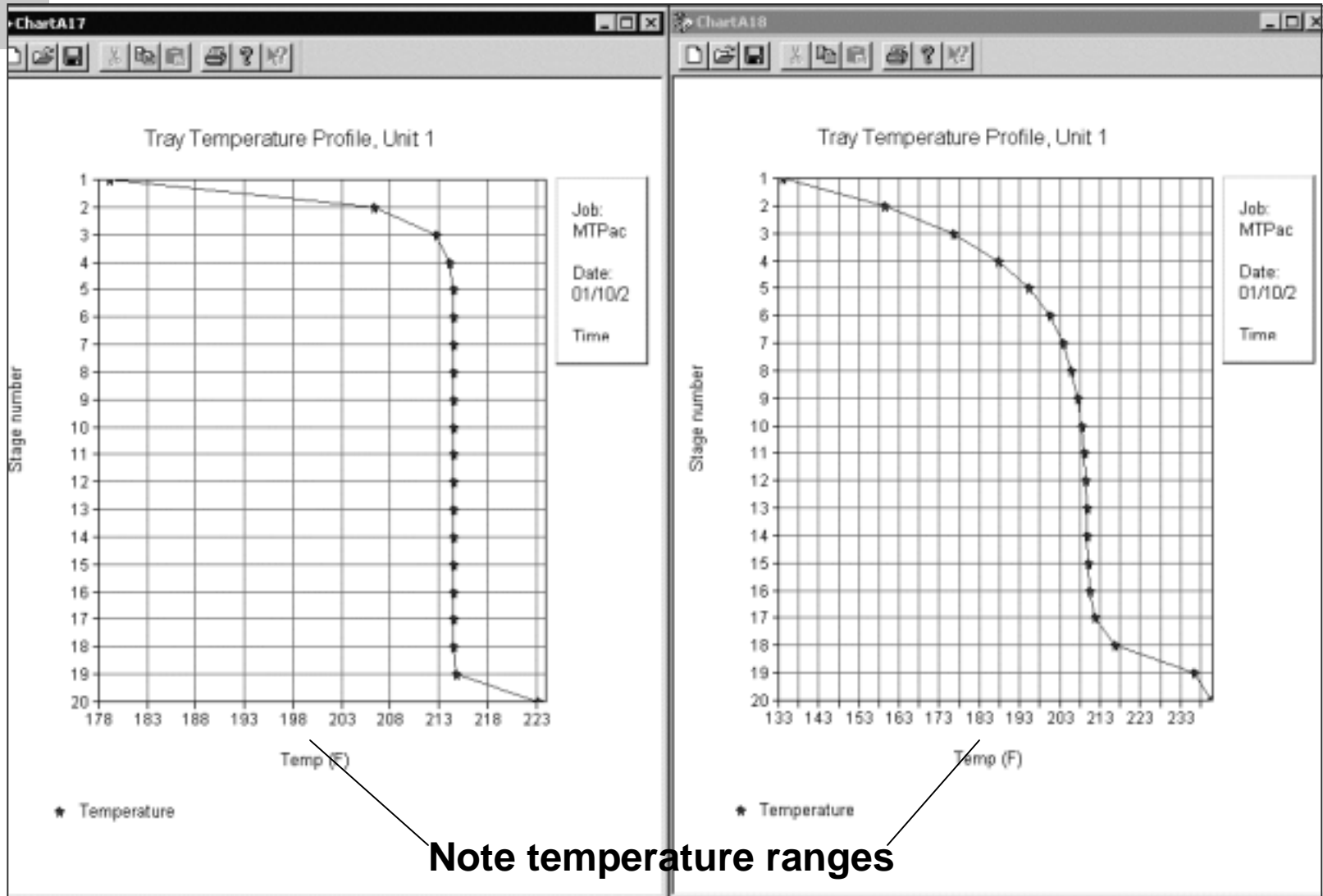
HCl Scrubbing:

Packed column mass transfer



Stream No.	1	2	3	4
Name				
- - Overall - -				
Molar flow lbmol/hr	251.0000	130.0000	116.6215	264.3785
Mass flow lb/hr	4540.2109	3974.9302	3180.4668	5334.6743
Temp F	100.0000	100.0000	179.0061	223.1575
Pres psia	50.0000	50.0000	50.0000	50.0000
Vapor mole fraction	0.0000	1.000	1.000	0.0000
Enth MMBtu/hr	-30.710	-1.1717	-1.6467	-30.235
Actual vol ft3/hr	73.4892	15572.6572	15957.3486	111.7490
Std liq ft3/hr	72.8439	74.1990	58.3214	88.7215
Std vap 60F scfh	95249.1328	49332.2227	44255.3789	100325.9922

HCI Scrubbing:





Mass Transfer in Distillation Calculations (cont.)

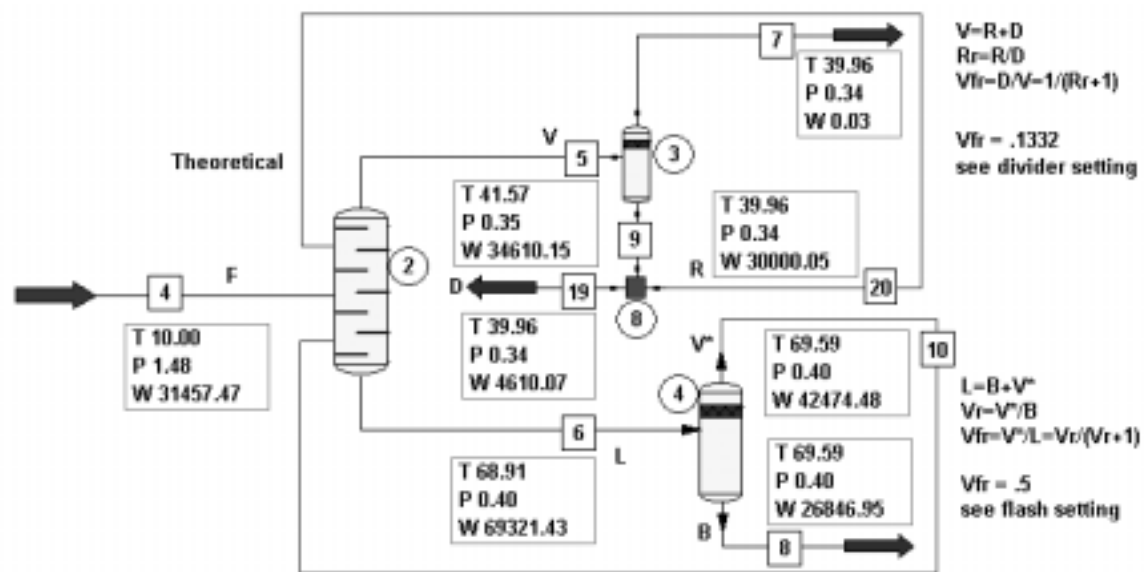
The rate-based approach is recommended for modeling of the following operations:

- Packed columns
- Mixtures which exhibit strongly non-ideal behavior
- Reactive distillation
- Any column with profiles of rapidly changing slope

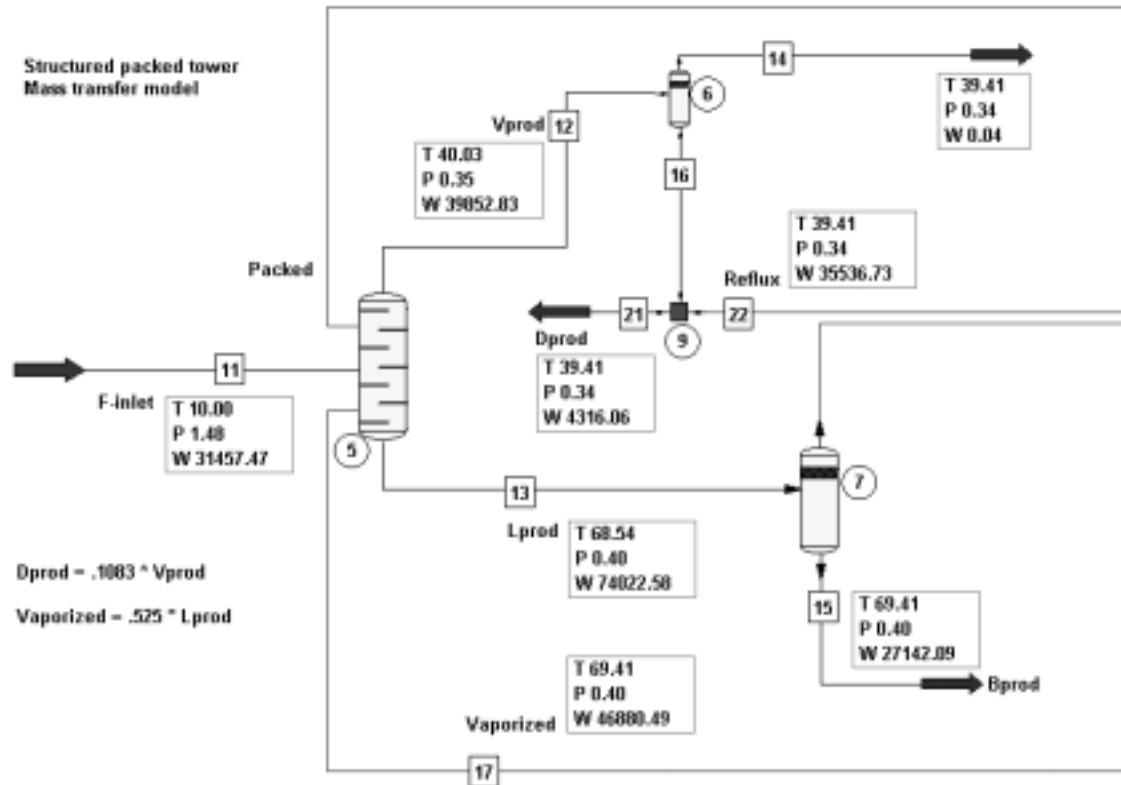


Thank You ...

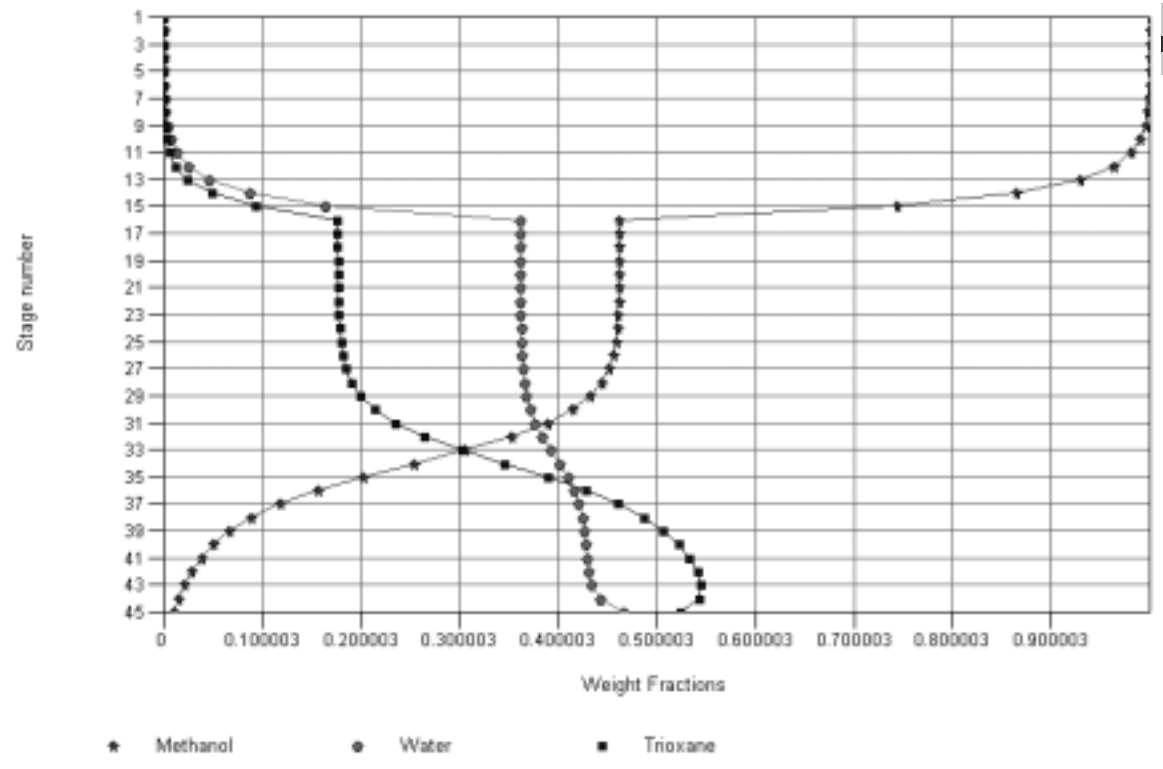
End



Structured packed tower
Mass transfer model



Tray Liquid Profile, Unit 5



Tray Temperature Profile, Unit 5

